A mesh refinement study on FCC polycrystalline aggregates with length scale effects

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Abstract

Strain gradient plasticity concepts are commonly used to study the effect of length scales in polycrystalline metal aggregates (ie. 'Hall-Petch' type behavior). Strain gradients arise primarily due to the incompatibility in deformation between neighboring grains, resulting in additional strengthening. This additional strengthening mechanism associated with these strain gradients are caused by the presence of geometrically-necessary dislocations (GNDs). Polycrystalline aggregates with finer structures create steeper strain gradients across grain boundaries, thus producing higher stress-strain responses due to the GNDs.

Here, a global mesh refinement study is conducted on a Cu polycrystalline aggregate. The study reveals that the rate of convergence of the predicted response of the aggregate (for a given strain) changes with decreasing length scales as the mesh is refined and may possibly diverge.

- In this work, a recently formulated dislocation density-based, gradient and rate-dependent crystallographic model is used to perform a global mesh refinement study on a Cu polycrystalline aggregate.
- The main objective of this study on a polycrystalline aggregate is to address the issue on the effect of decreasing length scales on the finite element convergence rate for a length scale dependent constitutive model.

General Framework :

- The single crystal formulation relies on the multiplicative decomposition of the deformation gradient, F into its inelastic component F^p and elastic component F^e.

$$F = F^e F^p$$

- Through the kinematics of dislocation motion, the rate of change of the inelastic deformation tensor is expressed as :

$$\dot{F}^p = \left\{ \sum_{\alpha} \dot{\gamma}^{\alpha} m^{\alpha} \otimes n^{\alpha} \right\} F^p$$

- The flow rule for an arbitrary slip system (α) is given as :

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \exp\left[-\frac{F_0}{k\theta} \left\langle 1 - \left\{ \frac{\tau^{\alpha} - S^{\alpha}\, \mu/\mu_0}{\hat{\tau}_0\, \mu/\mu_0} \right\}^p \right\rangle^q \right] \operatorname{sgn}(\tau^{\alpha})$$

Dislocation Density Model :

- The additional strengthening associated with the presence of strain gradients is due to the presence of geometrically-necessary dislocations (GNDs). Its density evolution is based on Nye's tensor in terms of the spatial gradient of the slip rate [1,2].

$$b_G^{\alpha}\left(\dot{\rho}_{Gs}^{\alpha} m^{\alpha} + \dot{\rho}_{Get}^{\alpha} t^{\alpha} + \dot{\rho}_{Gen}^{\alpha} n^{\alpha} \right) = curl.\left\{ \dot{\gamma}^{\alpha} n^{\alpha} F^p \right\} \quad \text{..............} (\Psi)$$

- The statistically stored dislocations (SSDs) are also discretized into pure edge and screw types.

$$\dot{\rho}_e^{\alpha} = \frac{C_e}{b_e^{\alpha}} \left(h_e \sqrt{\sum_{\beta=1}^{N} \delta^{\alpha\beta} \rho^{\beta}} - 2 f_e d_e \rho_e^{\alpha} \right) \left| \dot{\gamma}^{\alpha} \right|$$

$$\dot{\rho}_{sw}^{\alpha} = \frac{C_{sw}}{b_{sw}^{\alpha}} \left(h_{sw} \sqrt{\sum_{\beta=1}^{N} \delta^{\alpha\beta} \rho^{\beta}} - f_{sw} \rho_{sw}^{\alpha} \left\{ h_{sw} \pi d_{sw}^2 \sqrt{\sum_{\beta=1}^{N} \delta^{\alpha\beta} \rho^{\beta}} + 2 d_{sw} \right\} \right) \left| \dot{\gamma}^{\alpha} \right|$$

- *The physical model parameters are* $h_e, h_{sw}, d_e, d_{sw}, C_e, C_{sw}$

$$d_e = 1.0\ nm\ ;\ d_{sw} = 5.0\ nm\ ;\ h_e = h_{sw}/2\ ;\ C_e = C_{sw} = 0.5$$

FE model of the polycrystalline aggregate :

- Two polycrystalline aggregates described by representative volume elements (RVEs) with 8 and 64 randomly oriented grains are used in this study. They are herein, identified as *RVE8* and *RVE64* respectively.
- The stereographic projections of the random orientations in both RVEs can be seen in Figs. 1(a) and (b).
- Three different grain sizes of D=7.5, 15 and 150μm are considered in the study. The focus here is on monotonic loading applied in the x_3-direction at a low homologous temperature (ie. 22°C) and a strain rate of $10^{-3} s^{-1}$.
- The FE geometries used have a cubic geometry (Fig. 2 refers) and periodic boundary conditions are applied on the cube faces.
- The element type used here is a standard 20 node quadratic isoparametric brick element with reduced (2x2x2) integration.
- The evolution of the GNDs are calculated using the slip rate gradient terms in Eq.(Ψ) above. Here, the slip rate gradients are obtained through interpolation using an 8-node brick element with full (2x2x2) integration.

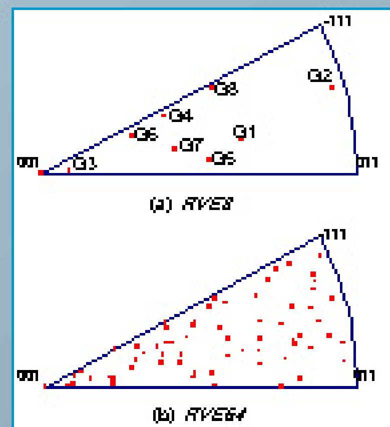


Fig. 1 - Stereographic projection of random grain orientations in the RVEs

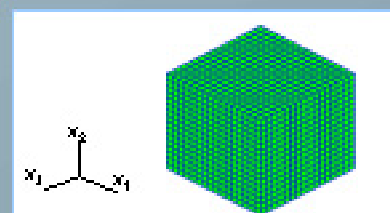
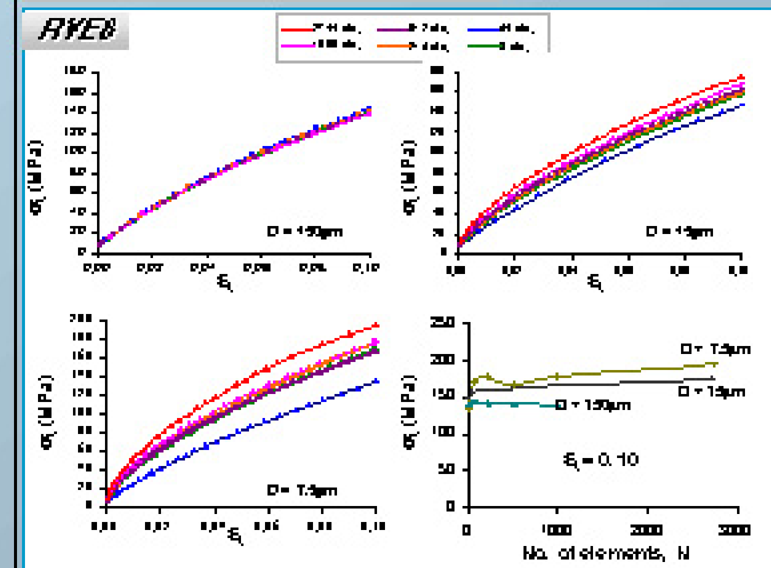
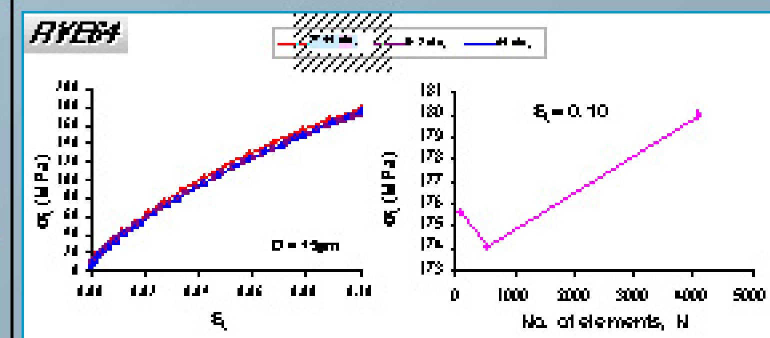


Fig. 2 – Generic FE model for both RVEs

Results :





Conclusions & Remarks:

- The mesh refinement study conducted reveals that, for an RVE with a small number of grains (*RVE8*) with a sufficiently large grain size (D=150μm), the response of the polycrystalline aggregate converges as the finite element mesh is refined.
- It was also revealed that the macroscopic response does not converge as the grain size was subsequently reduced by factors of 10 and 20.
- For a smaller grain size (ie. D=15μm), the study on an aggregate with a larger number of grains (*RVE64*) also indicates that the macroscopic response did not converge as the mesh was refined.
- The study indicates that with decreasing length scales, the polycrystalline aggregate response fails to converge with mesh refinement.

References :

1. Dai, H., Parks, D. M., 1997. Geometrically-necessary dislocation density and scale-dependent crystal plasticity. *In: Khan, A. (Ed.), Proceedings of Sixth International Symposium on Plasticity*. Gordon & Breach, pp 17-18

2. Busso, E. P., Meissonnier, F. T. and O'Dowd, N.P., Gradient-dependent deformation of precipitated single crystals. *J. Mech. Phys. Solids*, V 48 (2000), 2333-2361